**Coupled Harmonic Oscillators**

This is a reprisal of the content of corresponding files in the Classical Mechanics folder.

**Properties/Symmetries of K**

Okay, so first, let’s recall K’s primary definition:



And we can observe that due to equality of cross-partials, we have:



If we have a periodic crystal, then we should be able to make the mapping xα(**R**i) → xα(**R**i + **a**), where **a** is any lattice vector which points from one lattice site to another, without fundamentally changing anything – in particular, the energy. That is to say, we can replace the displacement of every atom with the displacement of the atom **a** away from it, w/o changing the energy. This implies,



Now this must be true for all xi(α) and xj(β). And this means we must have, for every **Ri**, **R**j:



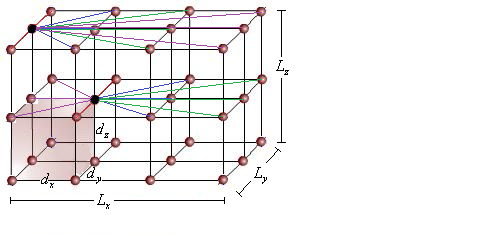
But say we made **a** = **R**j. Then we’d have:



Therefore **K** is a function only of the relative displacement of the ions. So we can write:



Quick note on Kαβ(**Ri**-**R**j). For fixed **R**j, there are N possible values for Kαβ(**R**i – **R**j). But it would seem that the set of possible values Kαβ(**R**i – **R**j) can take on would be depend on what **R**j is. But that’s not actually so, thanks to the periodicity condition. Consider a lattice below, and the two black atoms in particular. The colored lines are position vectors. And identical colors are identical sets. So in particular, the purple ones which up top traverse the entire crystal are equivalent to the purple ones in the middle which go backwards one unit cell.



Okay, moving on, we can say that every (repeating) crystal lattice has an inversion center so that if take that point as our origin, and make the mapping xα(**R**i) → -xα(-**R**i), we will end up with the same crystal and displacements, relative to each other. And so the potential energy won’t change under such a transformation. So that means:



Since this must be true for every xi(α), xj(β), it follows that we must have:



which, in light of the previous equality, means,



And so **K** is a symmetric matrix. There are a few other properties of note. If we translate all the ions a uniform displacement, **a**, this shouldn’t change the energy, as the relative orientations of the ions wouldn’t have changed. We can see what the consequence of this is for our **K**. Technically, **a** will have to be a small displacement, since our expansion of V is only good in a small neighborhood about all the **R**’s, out to second order in **x** (we’re not translating the equilibrium positions of the atoms, just the atoms themselves). So we should have:



Since this should be true for any **a**, and **x** for that matter, we must have:



There should also be rotational symmetry – i.e., if we rotate all particles by an angle **θ**, this shouldn’t change the energy, as it wouldn’t change the relative orientations of the particles. Our angle **θ** must be small, since again our V approximation is only good to second order in **x** (we’re not rotating the equilibrium positions of the atoms, just the atoms themselves). If we rotate the atoms in the crystal by θ, then the positions of all the particles will change to **r**i → **r**i + **r**i× → **x**i → **x**i + (**R**i+**x**i)× **≈ xi** + **R**i× (since x is first order, we can only keep terms to first order to be self-consistent). Well filling this into V, we have:



This must be zero for all **x**’s, and all **θ**’s. Everything will be zero if we just require:



We can leave it like this, or if we place our origin at **R**i, then we can write this as:



which looks slightly prettier. Now let’s consider **K**(q):



And consider two properties of Kαβ(q). First,



And second, we said Kαβ(**R**) = Kαβ(-**R**). And so we can say,



So this makes **K**(q) a real matrix. Further, it is symmetric, as we saw. And this guarantees that it has real eigenvalues. The eigenvalues have to be positive too, in order for the potential to be ‘concave up’. Else, the potential landscape would be a relative maximum, instead of minimum. So these are the main properties of concern for Kαβ(Ri,Rj) and Kαβ(q). Note this means that Kαβ(q) has only 6 d.o.f., since it’s a real symmetric matrix. Last thing. Note that:



So we can use these symmetries to write Kαβ(q) in a nice way,



So we have, making cosmetic change **R** → Δ**R**.



Well I guess we can exclude the ΔR=0 term from the sum, since we get zero. So,



**General formula for Potential Energy given pair-wise interaction**

Let’s say our ionic potential energy comes from the sum of some pair-wise potential, like the Coulomb potential for instance. Then we can say in general,



And we’d like to work out what V is to 2nd order in fluctuations about the equilibrium points. Let these be **R**Ri, and write **r**i = **R**i + **x**i. Then we can expand the two-body potential energy term as... (there is implicit summation over i, j, k, m)



Continuing,



So the total potential energy of our guys would be, presuming the Φ´ terms add up to zero, as it should in equilibrium:



Let’s define,



Then can write:



We can put this in HO form,



We can verify that this formula for K satisfies all the properties enumerated in previous file. For instance, consider the translational symmetry property. We’re supposed to have:



So that checks out. And consider the rotational symmetry property.



And this checks out, since any vector crossed into itself is zero. And we don’t use Ri as the origin, but shift it by some **a**, we still get zero, since:



**Direct Evaluation of K for Potential Energy with pair-wise form**

Let’s do same thing a different way. Recall we said,



where V is the total potential energy. Let Φ be the some pair-wise potential energy between neighbors. And let the interaction extend over all neighbors. Then we would have,



and,



And let’s work this out,



Guess I have to do that sum now. Luckily for us, we can extend the sum to include i = j terms because those are zero. So,



which gives us,



This matches the form of the result we had above.

